

Table D5. Individual hydrocarbon and total petroleum hydrocarbon concentrations (in µg/g wet wt.) for ribbed mussels taken from Old Place marsh, a replanted site.¹⁻³

Sample ID	Nonane (n-C ₉)	Decane (n-C ₁₀)	Undecane (n-C ₁₁)	Dodecane (n-C ₁₂)	Tridecane (n-C ₁₃)	Tetradecane (n-C ₁₄)	Pentadecane (n-C ₁₅)	Hexadecane (n-C ₁₆)	Heptadecane (n-C ₁₇)	Pristane	Octadecane (n-C ₁₈)	Phytane	Nonadecane (n-C ₁₉)	Eicosane (n-C ₂₀)	Heneicosane (n-C ₂₁)	Docosane (n-C ₂₂)	Tricosane (n-C ₂₃)
First Collection																	
197020410	nd	nd	nd	nd	nd	nd	nd	nd	0.17	0.12	nd	nd	nd	nd	1.25	nd	nd
197020411	2.67	nd	nd	nd	nd	nd	nd	nd	0.15	0.12	nd	nd	0.16	nd	1.60	nd	nd
197020412	0.50	nd	nd	nd	nd	nd	nd	nd	0.11	nd	nd	nd	0.22	nd	1.59	nd	nd
197020413	0.76	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	1.36	nd	nd
197020414	0.43	nd	nd	nd	nd	nd	nd	nd	0.18	0.12	nd	nd	nd	nd	1.32	nd	nd
Average⁴	0.90	nd	nd	nd	nd	nd	nd	nd	0.13	< MDL	nd	nd	< MDL	nd	1.43	nd	nd
Std Dev	1.02	-	-	-	-	-	-	-	0.06	-	-	-	-	-	0.16	-	-
Second Collection																	
497051411	0.31	nd	nd	nd	nd	nd	nd	nd	0.67	nd	nd	0.10	0.30	0.54	1.05	1.35	nd
497051412	nd	nd	nd	nd	nd	nd	nd	nd	0.32	0.11	nd	nd	0.13	nd	0.65	nd	nd
497051413	nd	nd	nd	nd	nd	nd	nd	nd	0.28	nd	nd	nd	nd	nd	0.56	nd	nd
497051414	nd	nd	nd	nd	nd	nd	nd	0.13	0.57	0.17	nd	0.17	nd	0.36	nd	1.79	nd
497051415	nd	nd	nd	nd	nd	nd	nd	nd	0.25	nd	nd	0.10	nd	nd	nd	nd	nd
Average⁴	< MDL	nd	nd	nd	nd	nd	nd	< MDL	0.42	< MDL	nd	< MDL	0.12	0.24	0.53	0.83	nd
Std Dev	-	-	-	-	-	-	-	-	0.19	-	-	-	0.10	0.20	0.36	0.69	-
MDL	0.24	0.06	0.12	0.12	0.11	0.11	0.11	0.09	0.08	0.10	0.10	0.10	0.11	0.21	0.38	0.68	2.47

Table D5. Continued.¹⁻³

Sample ID	Tetracosane (n-C ₂₄)	Pentacosane (n-C ₂₅)	Hexacosane (n-C ₂₆)	Heptacosane (n-C ₂₇)	Octacosane (n-C ₂₈)	Nonacosane (n-C ₂₉)	Triacotane (n-C ₃₀)	n-Hentriacontane (n-C ₃₁)	Dotriacontane (n-C ₃₂)	Tritriacontane (n-C ₃₃)	Tettriacontane (n-C ₃₄)	Pentatriacontane (n-C ₃₅)	Hexatriacontane (n-C ₃₆)	Heptatriacontane (n-C ₃₇)	Octatriacontane (n-C ₃₈)	Nonatriacontane (n-C ₃₉)	Tetracontane (n-C ₄₀)
First Collection																	
197020410	nd	nd	nd	0.26	0.42	nd	nd	0.41	0.42	0.58	0.65	0.75	0.73	0.73	0.56	0.41	0.26
197020411	nd	nd	0.13	nd	nd	nd	nd	0.55	0.43	0.56	0.59	0.72	0.68	0.68	0.52	0.39	0.24
197020412	nd	nd	nd	0.19	0.33	nd	nd	0.40	0.38	0.54	0.55	0.64	0.63	0.57	0.50	0.35	0.22
197020413	nd	nd	0.12	nd	nd	nd	nd	0.52	0.55	0.76	0.75	0.84	0.76	0.73	0.59	0.42	0.25
197020414	nd	nd	nd	nd	nd	nd	nd	0.34	0.56	0.20	0.36	0.41	0.38	0.39	0.31	0.23	0.14
Average⁴	nd	nd	< MDL	0.11	0.21	nd	nd	0.44	0.47	0.53	0.58	0.67	0.64	0.62	0.49	0.36	0.22
Std Dev	-	-	-	0.10	0.15	-	-	0.08	0.08	0.20	0.15	0.16	0.15	0.14	0.11	0.08	0.05
Second Collection																	
497051411	nd	nd	nd	nd	nd	nd	nd	8.89	3.40	0.29	nd	nd	nd	nd	0.09	nd	nd
497051412	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd
497051413	nd	nd	0.12	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	0.09	nd	nd
497051414	nd	nd	0.12	nd	nd	nd	nd	nd	nd	nd	nd	nd	0.10	nd	0.12	0.07	nd
497051415	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd	nd
Average⁴	nd	nd	< MDL	nd	nd	nd	nd	1.82	0.73	< MDL	nd	nd	< MDL	nd	< MDL	< MDL	nd
Std Dev	-	-	-	-	-	-	-	3.95	1.49	-	-	-	-	-	-	-	-
MDL	0.29	0.27	0.11	0.08	0.20	0.56	0.48	0.11	0.14	0.11	0.09	0.10	0.10	0.18	0.08	0.06	0.06

Table D5. Continued.¹⁻³

Sample ID	Total Petroleum Hydrocarbons ⁵	Total Concentrations of Individual Hydrocarbons ^{6,7,15}	Total: Pristane + Phytane ^{6,15}	Pristane/n-C ₁₇ ¹⁶	Phytane/n-C ₁₈ ¹⁶	Pristane/Phytane ¹⁶	Total: Odd No Carbons ^{6,8,15}	Total: Even No Carbons ^{6,9,15}	Carbon Preference Index (CPI) ^{10,16}	Sum: C ₁₀ -C ₁₂ -C ₁₄ ^{6,11,15}	Sum: C ₂₂ -C ₂₄ -C ₂₆ -C ₂₈ ^{6,12,15}	Weathering Index (WI) ^{13,16}
First Collection												
197020410	203	10.9	nd	0.73	-	-	6.55	4.16	1.57	nd	nd	-
197020411	158	13.3	nd	0.84	-	-	9.32	3.77	2.48	nd	nd	-
197020412	165	10.8	nd	-	-	-	6.92	3.73	1.86	nd	nd	-
197020413	106	11.6	nd	-	-	-	7.34	4.20	1.75	nd	nd	-
197020414	118	8.55	nd	0.63	-	-	5.42	2.97	1.82	nd	nd	-
Average⁴	150	11.0	nd	-	-	-	7.11	3.77	1.89 ¹⁷	nd	nd	-
Std Dev	39.1	1.70	-	-	-	-	1.43	0.49	-	-	-	-
Second Collection												
497051411	152	20.0	nd	-	-	-	13.5	6.29	2.15	nd	1.66	-
497051412	54.4	nd	nd	0.33	-	-	nd	nd	-	nd	nd	-
497051413	58.6	nd	nd	-	-	-	nd	nd	-	nd	nd	-
497051414	69.4	nd	0.34	0.29	-	0.96	nd	3.44	-	nd	2.16	-
497051415	nd	nd	nd	-	-	-	nd	nd	-	nd	nd	-
Average⁴	72.2	8.20	< MDL	-	-	-	5.18	< MDL	-	nd	< MDL	-
Std Dev	47.1	6.64	-	-	-	-	4.67	-	-	-	-	-
MDL	53.6	8.19 ¹⁴	0.19 ¹⁴				5.09 ¹⁴	2.91 ¹⁴		0.29 ¹⁴	1.29 ¹⁴	

Table D5. Continued.

Footnotes:

- ¹ The concentrations of the individual aliphatic hydrocarbons and the total petroleum hydrocarbons were determined using external standard calculations.
- ² When an individual aliphatic hydrocarbon was not detected, its concentration was replaced by nd.
- ³ The concentrations for n-C₈ will be not reported, since it was difficult to identify this peak in samples and to determine MDL for n-C₈.
- ⁴ If all concentrations are nd, the average is replaced with nd. When there is at least one number in the data set to be averaged, each nd is replaced with 1/2*MDL, and an average is calculated. If this numeric value is less than the MDL, the average is replaced by < MDL; otherwise, the average is the calculated value. When a numeric value is found for the average, the standard deviation is then determined using the same number set used to calculate the average.
- ⁵ Determined from the total peak areas in the chromatogram from n-C₈ to n-C₄₀ minus any contributions from the internal standard areas.
- ⁶ These formulae use 1/2MDL values for each analyte not detected.
- ⁷ Sum of the concentrations of the individual aliphatic hydrocarbons n-C₉ through n-C₄₀ plus the concentrations of pristane and phytane.
- ⁸ The total of the concentrations of the aliphatic hydrocarbons with an odd number of carbon atoms.
- ⁹ The total of the concentrations of the aliphatic hydrocarbons with an even number of carbon atoms. The contribution of n-C₈ is not included in the total.
- ¹⁰ Carbon Preference Index (CPI) defined as the ratio of the total of the concentrations of the aliphatic hydrocarbons with an odd number of carbons to the total concentration of the aliphatic hydrocarbons with an even carbon number.
- ¹¹ The total of the concentrations of n-C₁₀, n-C₁₂, and n-C₁₄.
- ¹² The total of the concentrations of n-C₂₂, n-C₂₄, n-C₂₆, and n-C₂₈.
- ¹³ Weathering Index (WI) is defined as the ratio of the total concentration of n-C₁₀, n-C₁₂, and n-C₁₄ to the total concentration of n-C₂₂, n-C₂₄, n-C₂₆, and n-C₂₈.
- ¹⁴ These MDL values are calculated with the same summation formulae as the samples using the individual hydrocarbon MDL values.
- ¹⁵ The summation totals for the samples are compared with calculated MDL values obtained using the same summation formulae as the samples. When these sample totals were less than the total MDL, its value was replaced by nd. The averages and standard deviations for the totals were treated in the same way as the individual hydrocarbons; see footnote 4.
- ¹⁶ Numerical values of the CPI, WI, and the ratios: pristane/n-C₁₇, phytane/n-C₁₈, and pristane/phytane, will be calculated only when the defined quantity for each index or ratio has a numeric value.
- ¹⁷ These results are not true averages, instead they are the ratios of the averages of the defined quantities, if these averages exist.